

The $\pi^0 - \eta - \eta'$ mixing in a generalized multi-quark interaction scheme.

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We investigate the isospin symmetry breaking effects within a recently derived Nambu-Jona-Lasinio related model by fitting the measured pseudoscalar meson masses and weak decay couplings f_π , f_K . Our model contains the next to leading order terms in the $1/N_c$ expansion of the effective multi-quark Lagrangian, including the ones that break the chiral symmetry explicitly. We show the important phenomenological role of these interactions: (1) they lead to an accurate fit of the low-lying pseudoscalar nonet characteristics; (2) they account for a very good agreement of the current quark masses with the present PDG values; (3) they reduce by 40% the ratio ϵ/ϵ' of the $\pi^0 - \eta$ and $\pi^0 - \eta'$ mixing angles, as compared to the case that contemplates explicit breaking only in the leading order, bringing it in consonance with the quoted values in the literature. The conventional NJL-type models fail in the joint description of these parameters.

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I. Introduction

The strong isospin symmetry is considered to be a very good approximation in the empirical description of a large bulk of strong interaction processes. This is related to the hierarchy in which breaking of the chiral symmetry $SU(3)_L \times SU(3)_R$ by different current quark masses occurs, down to $SU(2)_I \times U(1)_Y$ flavor symmetry if $m_u, m_d \ll m_s$. In the case of the pseudoscalar mesons it is accurate at the order of the ratio of the light and strange current quark masses $(m_u - m_d)/m_s$ [1],[2] and explains partly the small meson mass differences within charged isospin multiplets. A further source of isospin breaking is due to the electromagnetic interactions, which are expected to be suppressed at the scale of strong interactions.

A detailed quantitative analysis however requires isospin breaking corrections to be taken into account in a series of low energy phenomena, such as: the description of mass splittings of mesons, and Dashen's theorem [3]; sum rules for quark condensates [2], [4]; kaon decays [5]; $\pi - \pi$ [6],[7] and $\pi - K$ scattering [8],[9] in relation to mesonic atoms, [10],[11], ρ and τ decays involving $\eta(\eta')$ mesons [12], $a_0 - f_0$ mixing [13] in the scalar meson sector.

Strong isospin breaking effects become particularly relevant if a certain process depends crucially on the differences of the light quark masses. If in addition the electromagnetic interactions are a subleading effect, these processes provide for ideal tools in a quantitative analysis of quark mass ratios. In the latter category are the $\eta, \eta' \rightarrow 3\pi$ decays, the $\pi^0 - \eta$ and $\pi^0 - \eta'$ mixings, as well as the $\rho - \omega$ mixing in the vector channels.

Isospin breaking associated with the $\pi^0 - \eta - \eta'$ system has long been known to play a role in the Standard

Model prediction of the CP violation related ratio $(\frac{\epsilon'}{\epsilon})_{CP}$ [14–17] representing a substantial correction to the QCD penguin contributions [16]. It affects the value of the $K^0 \rightarrow \pi^0 \pi^0$ transition through the dominant QCD Q_6 penguin operator, which is one of the sources of uncertainties in the determination of $(\frac{\epsilon'}{\epsilon})_{CP}$ [18], for a recent review see [19].

In chiral perturbation theory (ChPT)[20],[21],[2] the $\pi^0 - \eta$ mixing angle occurs already at order p^2 and was first evaluated to order p^4 in the context of K_{l3} form factors in [21].

In the analysis of $\eta - \eta'$ mixing of [22] the $U(1)_A$ anomaly is described by the gluon transition matrix element $\langle 0 | \frac{\alpha_s}{4\pi} G\tilde{G} | \eta_i \rangle$ and the quark flavor basis has been used. As shown in [23] this basis is favored, as one of the two mixing angles is indeed small. The decay constants follow the pattern of particle state mixing in that basis. It has been shown that this approach leads to results consistent with many observables related to $\eta - \eta'$ mixing [22]. In [24],[25] it has been extended to include the mixing to the neutral pion.

In the present work we address the $\pi^0 - \eta - \eta'$ mixings resulting from a recently proposed Lagrangian [26],[27], which is reviewed below. In this effective Lagrangian approach built from all spin 0 and non-derivative multi-quark interactions relevant at the scale of spontaneous chiral symmetry breaking, the complete set of interactions which break explicitly the chiral symmetry was included for the first time. This Lagrangian represents a generalization of the original Nambu-Jona-Lasinio [28, 29] model extended to the realistic three flavor and color case with $U(1)_A$ breaking six-quark 't Hooft interactions [30–44] and an appropriate set of eight-quark interactions [45]. The last ones complete the number of vertices which are important in four dimensions for dynamical $SU(3)_L \times SU(3)_R$ chiral symmetry breaking [46, 47]. The Lagrangian considers all interactions relevant at the same order in large N_c counting as the $U(1)_A$ anomaly term.

The role of the new interactions contained in the explicit symmetry breaking (ESB) vertices has been an-

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alyzed at meson tree level approximation and in the isospin limit in connection with the low lying characteristics of the pseudoscalar and scalar meson nonets [26],[27] and in the $T - \mu$ phase diagram associated with chiral transitions [48]. An unprecedented accuracy for the description of the spectra has been achieved. One should stress that the present Lagrangian is able to account properly for the $SU(3)$ breaking effects in the description of the weak decay constants f_π and f_K , in addition to yield the correct empirical η , η' and K meson masses, as well as the anomalous two photon decays of π, η, η' , in an unified description, which was an open problem for model versions without the ESB terms.

The paper is organized as follows. In the next section is presented the effective multiquark Lagrangian and its bosonized form, the associated N_c counting is reviewed, in section III we address the mixing in the $\pi - \eta - \eta'$ system, the choices of representation of states, the decay parameters in the flavor basis, and the compliance of the model in the approximation considered with the decay parameters transforming as the states. In section IV we present and discuss the numerical fits of the mass spectra and decay parameters. We end with a summary of the main results.

II. Survey of the model Lagrangian

II a. Multiquark picture

The Langrangian considered is built from all spin 0 chiral $SU(3)_L \times SU(3)_R$ symmetric and parity conserving combinations relevant at the scale Λ of spontaneous breaking of chiral symmetry. This means that in the corresponding effective potential are kept all the interactions which do not vanish in the $\Lambda \rightarrow \infty$ limit. These consist of vertices involving non-derivative quark-antiquark fields, denoted by Σ , with $\Sigma = \frac{1}{2}(s_a - ip_a)\lambda_a$ and $s_a = \bar{q}\lambda_a q$, $p_a = \bar{q}i\gamma_5\lambda_a q$, λ_a being the standard Gell-Mann matrices for $a = 1..8$ and $\lambda_0 = \sqrt{2/3} \times 1$, as well as of their interactions with the external sources χ which transform as $\chi = (3, 3*)$ under $SU(3)_L \times SU(3)_R$,

$$L = \bar{q}i\gamma^\mu \partial_\mu q + L_{int} + L_\chi. \quad (1)$$

The term

$$\begin{aligned} L_{int} = & \frac{\bar{G}}{\Lambda^2} \text{tr}(\Sigma^\dagger \Sigma) + \frac{\bar{\kappa}}{\Lambda^5} (\det \Sigma + \det \Sigma^\dagger) \\ & + \frac{\bar{g}_1}{\Lambda^8} (\text{tr} \Sigma^\dagger \Sigma)^2 + \frac{\bar{g}_2}{\Lambda^8} \text{tr}(\Sigma^\dagger \Sigma \Sigma^\dagger \Sigma). \end{aligned} \quad (2)$$

is well known. Here and elsewhere we use barred quantities for any dimensionless coupling, these are related to the dimensionful ones through powers of the scale Λ , $g_i = \bar{g}_i/\Lambda^\gamma$. L_{int} contains the leading order (LO) in N_c four quark (q) NJL interactions with coupling \bar{G} , generalized to the 3 flavor case, the NLO 6q 't Hooft $U(1)_A$ breaking flavor determinant with coupling $\bar{\kappa}$, and the two possible 8q interactions $\sim \bar{g}_1, \bar{g}_2$, which have the same N_c counting as the 't Hooft term. We refer to [26],[27] for

a detailed discussion of the large N_c counting scheme which complies with the counting rules based on powers of the scale Λ of spontaneous breaking of chiral symmetry. Rephrasing it, means that the terms which vanish as $\Lambda \rightarrow \infty$ are the same that also vanish on grounds of $N_c \rightarrow \infty$. Applying these rules, summarized after eq. 4, the following set of terms involving interactions with the sources χ emerge, which act also up to the same order in N_c counting as the 't Hooft term

$$L_\chi = \sum_{i=0}^{10} L_i, \quad (3)$$

where

$$\begin{aligned} L_0 &= -\text{tr}(\Sigma^\dagger \chi + \chi^\dagger \Sigma) \\ L_1 &= -\frac{\bar{\kappa}_1}{\Lambda} e_{ijk} e_{mnl} \Sigma_{im} \chi_{jn} \chi_{kl} + h.c. \\ L_2 &= \frac{\bar{\kappa}_2}{\Lambda^3} e_{ijk} e_{mnl} \chi_{im} \Sigma_{jn} \Sigma_{kl} + h.c. \\ L_3 &= \frac{\bar{g}_3}{\Lambda^6} \text{tr}(\Sigma^\dagger \Sigma \Sigma^\dagger \chi) + h.c. \\ L_4 &= \frac{\bar{g}_4}{\Lambda^6} \text{tr}(\Sigma^\dagger \Sigma) \text{tr}(\Sigma^\dagger \chi) + h.c. \\ L_5 &= \frac{\bar{g}_5}{\Lambda^4} \text{tr}(\Sigma^\dagger \chi \Sigma^\dagger \chi) + h.c. \\ L_6 &= \frac{\bar{g}_6}{\Lambda^4} \text{tr}(\Sigma \Sigma^\dagger \chi \chi^\dagger + \Sigma^\dagger \Sigma \chi^\dagger \chi) \\ L_7 &= \frac{\bar{g}_7}{\Lambda^4} (\text{tr} \Sigma^\dagger \chi + h.c.)^2 \\ L_8 &= \frac{\bar{g}_8}{\Lambda^4} (\text{tr} \Sigma^\dagger \chi - h.c.)^2 \\ L_9 &= -\frac{\bar{g}_9}{\Lambda^2} \text{tr}(\Sigma^\dagger \chi \chi^\dagger \chi) + h.c. \\ L_{10} &= -\frac{\bar{g}_{10}}{\Lambda^2} \text{tr}(\chi^\dagger \chi) \text{tr}(\chi^\dagger \Sigma) + h.c. \end{aligned} \quad (4)$$

We recall that the N_c book keeping is as follows:

$$\begin{aligned} \Sigma &\sim N_c, \quad \Lambda \sim N_c^0 = 1, \quad G \sim 1/N_c, \quad \kappa \sim 1/N_c^3, \\ \kappa_1, g_9, g_{10} &\sim 1/N_c, \\ \kappa_2, g_5, g_6, g_7, g_8 &\sim 1/N_c^2, \quad g_3, g_4 \sim 1/N_c^3. \end{aligned} \quad (5)$$

The scale Λ which gives the right dimensionality to the multiquark vertices is related with the cutoff on the divergent quark one-loop integrals, its N_c counting is dictated by the gap equations in the phase of spontaneously broken chiral symmetry, eqs. (21),(22),(23) below.

The terms $L_1 \dots L_{10}$ of Lagrangian (4) have been introduced recently in the model [26],[27] and generalize to NLO in N_c the explicit symmetry breaking (ESB) standard LO mass term L_0 .

Since all the blocks $L_0 \dots L_{10}$ conform with the symmetry pattern of the model one is free to choose for the source the constant valued matrix $\chi = \mathcal{M}/2$,

$$\mathcal{M} = \mu_a \lambda_a = \text{diag}(\mu_u, \mu_d, \mu_s). \quad (6)$$

TABLE I: The pseudoscalar masses and weak decay constants (all in MeV) in the isospin limit used as input (marked with *) for different sets of the model. Parameter sets (a),(b) contain explicit symmetry breaking interactions (see Table III) and allow for a fit of the scalar masses and strong decays as well, $m_\sigma = 550$ MeV, $m_\kappa = 850$ MeV, $m_{a_0} = m_{f_0} = 980$ MeV [27]; set (c) does not. Set (a) corresponds to an octet-singlet mixing angle in the scalar sector of $\theta_S = 27.5^\circ$, set (b) to $\theta_S = 25^\circ$.

Sets	m_π	m_K	m_η	$m_{\eta'}$	f_π	f_K
a	138*	494*	547*	958*	92*	113*
b	138*	494*	547*	958*	92*	113*
c	138*	494*	475*	958*	92*	115.7

TABLE II: Parameter sets of the model: $m_u = m_d = \hat{m}$, m_s , and Λ are given in MeV. The couplings have the following units: $[G] = \text{GeV}^{-2}$, $[\kappa] = \text{GeV}^{-5}$, $[g_1] = [g_2] = \text{GeV}^{-8}$. We also show here the values of constituent quark masses $M_u = M_d = \hat{M}$ and M_s in MeV. See also caption of Table I.

Sets	\hat{m}	m_s	\hat{M}	M_s	Λ	G	$-\kappa$	g_1	g_2
a	4.0*	100*	373	544	828	10.48	122.	3284	173
b	4.0*	100*	372	542	829	9.83	118.5	3305	-158
c	6.1	190	375	569	836	9.79	138.2	2500*	100*

TABLE III: Explicit symmetry breaking interaction couplings. The couplings have the following units: $[\kappa_2] = \text{GeV}^{-3}$, $[g_3] = [g_4] = \text{GeV}^{-6}$, $[g_5] = [g_6] = [g_7] = [g_8] = \text{GeV}^{-4}$. See also caption of Table I.

Sets	κ_2	$-g_3$	g_4	g_5	$-g_6$	$-g_7$	g_8
a	6.17	6497	1235	213	1642	13.3	-64
b	5.61	6472	702	210	1668	100	-38
c	0	0	0	0	0	0	0

TABLE IV: The mixing angles in the $\eta - \eta'$ system in isospin limit, and related weak decay constants for the sets discussed and in comparison with different approaches, see also main text (the systematic error estimates given in [81],[83] have been omitted here).

Sets	θ_P°	θ_0°	θ_8°	$\frac{f_0}{f_\pi}$	$\frac{f_8}{f_\pi}$
a	-12*	-1.42	-21.37	1.172	1.318
b	-15*	-4.42	-24.37	1.172	1.322
c	-14.5	-2.82	-24.78	1.197	1.365
[22] phen.	-13.3	-6.8	-19.4	1.10	1.19
[22] phen.	-15.4	-9.2	-21.2	1.17	1.26
[79] CHPT	-10.5	-1.5	-20.0	1.24	1.31
[54] CHPT	-	-4.	-20.5	1.10	1.28
[80] sum rules	-	-15.6	-10.8	1.39	1.39
[81] Padé approximants (η)	-16.4	-11.3	-21.3	1.15	1.22
[81] Padé approximants (η')	-13.3	-1.5	-24.2	1.28	1.46
[83] BABAR (from [81] (η))	-21.7	-26.7	-16.5	1.04	0.98
[83] BABAR (from [81] (η'))	-17.7	-15.6	-19.9	1.14	1.11

TABLE V: Empirical input used in the fits with isospin breaking, sets A and B with ESB interactions, set C without. Primes indicate which masses of the pion and kaon multiplets have been used for the fit, the other being output. Masses in units of MeV, angle ψ in degrees.

Sets	m_π^0	m_π^\pm	m_η	m'_η	m_K^0	m_K^\pm	f_π	f_K	ψ
A,B	136'	136.6	547	958	500	494'	92	113	39.7
C	136'	137.0	477	958	501	497'	92	116	39.7

TABLE VI: Parameter sets with isospin breaking, set A with ESB interactions, set B without. The couplings have the following units: $[G] = \text{GeV}^{-2}$, $[\kappa] = \text{GeV}^{-5}$, $[g_1] = [g_2] = \text{GeV}^{-8}$, $[\kappa_2] = \text{GeV}^{-3}$, $[g_3] = [g_4] = \text{GeV}^{-6}$, $[g_5] = [g_6] = [g_7] = [g_8] = \text{GeV}^{-4}$. Λ is given in MeV. See also caption of Table I.

Sets	G	$-\kappa$	g_1	g_2	Λ	κ_2	g_3	g_4	g_5	g_6	g_7	g_8
A	10.48	116.8	3284	1237	828.5	6.24	2365	1182	160	712	580	44
B	10.48	116.8	3284	1252	828.5	6.26	2481	1182	151	745	591	49
C	9.79	137.4	2500	117	835.7	0	0	0	0	0	0	0

TABLE VII: Isospin breaking parameter $r = \frac{m_d - m_u}{m_d + m_u}$, current and constituent quark masses m_u , m_d, m_s , M_u , M_d , M_s in MeV and $\pi^0 - \eta$, $\pi^0 - \eta'$ mixing angles ϵ and ϵ' .

Sets	r	m_u	m_d	m_s	M_u	M_d	M_s	ϵ	ϵ'	$\frac{\epsilon}{\epsilon'}$
A	0.372*	2.179	4.760	95*	372	375	544	0.014*	0.0037*	3.78
B	0.372*	2.166	4.733	95*	372	375	544	0.017*	0.0045*	3.95
C	0.372*	3.774	8.246	194	373	380	573	0.022	0.0025	8.78

Whenever convenient we use in the following the equivalent redefinition of flavor indices from $a = 0, 3, 8$ to $i = u, d, s$ for any observable A [49]

$$A_a = e_{ai} A_i, \quad e_{ai} = \frac{1}{2\sqrt{3}} \begin{pmatrix} \sqrt{2} & \sqrt{2} & \sqrt{2} \\ \sqrt{3} & -\sqrt{3} & 0 \\ 1 & 1 & -2 \end{pmatrix}. \quad (7)$$

The terms L_1, L_9, L_{10} are related to the Kaplan-Manohar ambiguity [50–53] in the definition of the quark mass. In the present case this corresponds to the following freedom in transforming the external source [26]

$$\begin{aligned} \chi^{(c_i)} = & \chi + \frac{c_1}{\Lambda} (\det \chi^\dagger) \chi (\chi^\dagger \chi)^{-1} + \frac{c_2}{\Lambda^2} \chi \chi^\dagger \chi \\ & + \frac{c_3}{\Lambda^2} \text{tr}(\chi^\dagger \chi) \chi \end{aligned} \quad (8)$$

with three independent constants c_i , which has the same symmetry transformation property as χ . The description in terms of $\chi^{(c_i)}$ in the place of χ is equivalent, leading to the same Lagrangian, with some of the couplings redefined as

$$\begin{aligned} \bar{\kappa}_1 \rightarrow \bar{\kappa}'_1 &= \bar{\kappa}_1 + \frac{c_1}{2}, \quad \bar{g}_5 \rightarrow \bar{g}'_5 = \bar{g}_5 - \bar{\kappa}_2 c_1, \\ \bar{g}_7 \rightarrow \bar{g}'_7 &= \bar{g}_7 + \frac{\bar{\kappa}_2}{2} c_1, \quad \bar{g}_8 \rightarrow \bar{g}'_8 = \bar{g}_8 + \frac{\bar{\kappa}_2}{2} c_1, \\ \bar{g}_9 \rightarrow \bar{g}'_9 &= \bar{g}_9 + c_2 - 2\bar{\kappa}_1 c_1, \\ \bar{g}_{10} \rightarrow \bar{g}'_{10} &= \bar{g}_{10} + c_3 + 2\bar{\kappa}_1 c_1. \end{aligned} \quad (9)$$

Note that the redefinition of the χ fields (8) in the model contains more terms than the one usually considered, in the context of second order ChPT, which leads to the following redefinition of the current quark mass [50]

$$\mathcal{M} \rightarrow \mathcal{M}(\lambda) = \mathcal{M} + \lambda \mathcal{M}(\mathcal{M}^\dagger \mathcal{M})^{-1} \det \mathcal{M}^\dagger. \quad (10)$$

It has been reported that the Kaplan-Manohar ambiguity may be in conflict with the large N_c counting rules of ChPT [54]. Following from a threefold chiral expansion in the number of derivatives, powers of quark masses

and powers of $1/N_c$, as well as the counting associated with the θ angle related with the $U_A(1)$ sector, λ is found to be suppressed to all orders in the large N_c limit [54].

Regarding our model Lagrangian, the new couplings, the primed ones in (9), must not dominate over the N_c dependence of the unprimed ones. This means that in their leading contributions they scale at most as the unprimed couplings, $c_i \sim 1/N_c$, see (5). Attributing this counting to the c_i suffices to warrant that one can use the reparametrization freedom (9), in particular to obtain $\bar{\kappa}'_1 = \bar{g}'_9 = \bar{g}'_{10} = 0$. Indeed, remembering that our model Lagrangian has been constructed to incorporate the classes of multiquark interactions which do not vanish in the effective potential as $N_c \rightarrow \infty$ in the phase of spontaneously broken chiral symmetry, one gets for this case that $\bar{\kappa}_1 = -c_1/2$, and that up to subleading corrections (not considered at this order of the effective potential), $\bar{g}_9 = -c_2, \bar{g}_{10} = -c_3, \bar{g}'_5 = \bar{g}_5, \bar{g}'_7 = \bar{g}_7, \bar{g}'_8 = \bar{g}_8$.

II b. Bosonized version

The low energy meson characteristic are obtained after path integral bosonization of the quark Lagrangian (1). Following [34] one may equivalently use the introduced s_a, p_a as auxiliary fields, and a further set of physical scalar and pseudoscalar fields $\sigma = \sigma_a \lambda_a, \phi = \phi_a \lambda_a$ to obtain the vacuum persistence amplitude of the theory as

$$\begin{aligned} Z = & \int \mathcal{D}q \mathcal{D}\bar{q} \prod_a \mathcal{D}\sigma_a \prod_a \mathcal{D}\phi_a \exp \left(i \int d^4x L_q(\bar{q}, q, \sigma, \phi) \right) \\ & \times \int_{-\infty}^{+\infty} \prod_a \mathcal{D}s_a \prod_a \mathcal{D}p_a \exp \left(i \int d^4x L_{aux}(\sigma, \phi; s, p) \right). \end{aligned} \quad (11)$$

In these variables the Lagrangian reads

$$L = L_q + L_{aux}$$

TABLE VIII: ϵ and ϵ' values in the literature.

	ϵ	ϵ'	$\frac{\epsilon}{\epsilon'}$
[63] phen.	0.014	0.0037	3.78
[25] phen.	0.017 ± 0.002	0.004 ± 0.001	4.25 ± 1.17
[79] ChPt NLO	$0.014 \div 0.016$	-	-
[84] phen.	0.021	-	-
[85] Exp.	0.030 ± 0.002	-	-
[86] Exp.	0.026 ± 0.007	-	-

$$\begin{aligned}
L_q &= \bar{q}(i\gamma^\mu\partial_\mu - (\sigma + M) - i\gamma_5\phi)q \\
L_{aux} &= s_a(\sigma_a + M_a - m_a) + p_a\phi_a + L_{int}(s, p) \\
&+ \sum_{i=2}^8 L'_i(s, p, m).
\end{aligned} \tag{12}$$

Here L'_i contains the ESB terms and L_0 appears as $s_a m_a$ in L_{aux} . The external scalar fields σ have been shifted to $\sigma \rightarrow \sigma + M$, so that the expectation value of the shifted fields in the vacuum corresponding to dynamically broken chiral symmetry vanish. The expectation value of the unshifted scalar field $\langle \sigma \rangle = M_a \lambda_a = \text{diag}(M_u, M_d, M_s)$ corresponds to the point where the effective potential of the theory achieves its minimum, with M being the constituent quark masses. In (12) the bilinear form in the quark fields L_q can be integrated out from the path integral, and results in the fermion determinant (see (18) below), which generates the kinetic terms of the σ, ϕ fields. The remaining integrations are over a static non-Gaussian system of s, p fields, and are done in the stationary phase approximation (SPA). First we present the results for the SPA integration, obtained from the extremum conditions

$$\frac{\partial L}{\partial s_a} = 0, \quad \frac{\partial L}{\partial p_a} = 0, \tag{13}$$

which must be fulfilled in the neighbourhood of the uniform vacuum state of the theory. The solutions of eq. (13) are sought in the form:

$$\begin{aligned}
s_a^{st} &= h_a + h_{ab}^{(1)}\sigma_b + h_{abc}^{(1)}\sigma_b\sigma_c + h_{abc}^{(2)}\phi_b\phi_c + \dots \\
p_a^{st} &= h_{ab}^{(2)}\phi_b + h_{abc}^{(3)}\phi_b\sigma_c + \dots
\end{aligned} \tag{14}$$

Eqs. (13) determine all coefficients of this expansion giving rise to a system of cubic equations to obtain h_a , eq. (16), and a full set of recurrence relations to find higher order coefficients in (14). The result is cast in the form

$$\begin{aligned}
L_{aux} &= h_a\sigma_a + \frac{1}{2}h_{ab}^{(1)}\sigma_a\sigma_b + \frac{1}{2}h_{ab}^{(2)}\phi_a\phi_b \\
&+ \frac{1}{3}\sigma_a \left[h_{abc}^{(1)}\sigma_b\sigma_c + \left(h_{abc}^{(2)} + h_{bca}^{(3)} \right) \phi_b\phi_c \right] + \dots
\end{aligned} \tag{15}$$

Here h_a are related to the quark condensates, $h_{ab}^{(1)}$, $h_{ab}^{(2)}$ contribute to the masses of scalar and pseudoscalar states respectively, and higher indexed h 's are the couplings

that measure the strength of the meson-meson interactions. From eq. (13) and using (7) one obtains the following system of cubic equations for the one index coefficients h_i , ($i = \{u, d, s\}$)

$$\begin{aligned}
M_i - m_i + \frac{\kappa}{4}t_{ijk}h_jh_k + \frac{h_i}{2}(2G + g_1h^2 + g_4mh) + \frac{g_2}{2}h_i^3 \\
+ \frac{m_i}{4}[3g_3h_i^2 + g_4h^2 + 2(g_5 + g_6)m_ih_i + 4g_7mh] \\
+ \kappa_2t_{ijk}m_jh_k = 0.
\end{aligned} \tag{16}$$

Here t_{ijk} is a totally symmetric quantity, whose nonzero components are $t_{uds} = 1$; there is no summation over the open index i but we sum over the dummy indices, e.g. $h^2 = h_u^2 + h_d^2 + h_s^2$, $mh = m_uh_u + m_dh_d + m_sh_s$. Regarding the h coefficients with more than one index, we indicate explicitly only the expression needed for the present study of the pseudoscalar masses (the complete expressions up to 3 indices can be found in [26],[27])

$$\begin{aligned}
-2\left(h_{ab}^{(2)}\right)^{-1} &= (2G + g_1h^2 + g_4mh)\delta_{ab} \\
-3A_{abc}(\kappa h_c + 2\kappa_2m_c) + g_2h_rh_c(d_{abe}d_{cre} + 2f_{are}f_{bce}) \\
+ g_3m_rh_c(d_{abe}d_{cre} + f_{are}f_{bce} + f_{ace}f_{bre}) \\
- g_5m_rm_c(d_{are}d_{bce} - f_{are}f_{bce}) \\
+ g_6m_rm_cd_{abe}d_{cre} - 4g_8m_am_b.
\end{aligned} \tag{17}$$

which can be readily inverted. These coefficients are totally defined in terms of h_a and the parameters of the model.

Now to the fermion determinant related to the integration over the fermion fields: we expand it using a heat-kernel technique that takes appropriately into account the quark mass differences, being chiral covariant at each order of the expansion [55–57],

$$\begin{aligned}
W[Y] &= \ln |\det D| = -\frac{1}{2} \int_0^\infty \frac{dt}{t} \rho(t) \exp \left(-tD_E^\dagger D_E \right), \\
D_E^\dagger D_E &= M^2 - \partial^2 + Y, \quad Y = i\gamma_\mu(\partial_\mu + i\gamma_5\partial_\mu\phi) \\
&+ \sigma^2 + \{M, \sigma\} + \phi^2 + i\gamma_5[\sigma + M, \phi],
\end{aligned} \tag{18}$$

or

$$W[Y] = - \int \frac{d^4x_E}{32\pi^2} \sum_{i=0}^{\infty} I_{i-1} \text{tr}[b_i] \tag{19}$$

where D_E stands for the Dirac operator in Euclidean space. We consider the expansion up to the third modified Seeley-DeWitt coefficient b_i

$$\begin{aligned} b_0 &= 1, \quad b_1 = -Y, \\ b_2 &= \frac{Y^2}{2} + \frac{\lambda_3}{2} \Delta_{ud} Y + \frac{\lambda_8}{2\sqrt{3}} (\Delta_{us} + \Delta_{ds}) Y, \end{aligned} \quad (20)$$

with $\Delta_{ij} = M_i^2 - M_j^2$. This order of the expansion takes into account the dominant contributions of the quark one-loop integrals I_i ($i = 0, 1, \dots$); these are the arithmetic average values $I_i = \frac{1}{3}[J_i(M_u^2) + J_i(M_d^2) + J_i(M_s^2)]$ where

$$J_i(m^2) = \int_0^\infty \frac{dt}{t^{2-i}} \rho(t\Lambda^2) e^{-tm^2}, \quad (21)$$

with the Pauli-Villars regularization kernel [58, 59]

$$\rho(t\Lambda^2) = 1 - (1 + t\Lambda^2) \exp(-t\Lambda^2). \quad (22)$$

which is equivalent to the sharp 4D cutoff regularization for the scalar integrals considered. Both terms proportional to b_1 and b_2 have contributions to the gap equations and meson masses, but only b_2 contributes to the kinetic and meson interaction terms. By excluding the σ tadpole from the total Lagrangian, one obtains the gap equations

$$h_i + \frac{N_c}{6\pi^2} M_i [3I_0 - (3M_i^2 - M^2) I_1] = 0. \quad (23)$$

where $M^2 = M_u^2 + M_d^2 + M_s^2$. We now see that (23) must be solved self-consistently with the SPA equations (16).

III. Mixing in the π^0, η, η' system

III a. Choices of representations

Finally one is ready to combine the terms of the total Lagrangian L that contribute to the kinetic terms L_{kin} and meson masses L_{mass}

$$\begin{aligned} &L_{kin} + L_{mass} \\ &= \frac{N_c I_1}{16\pi^2} \text{tr} [(\partial_\mu \sigma)^2 + (\partial_\mu \phi)^2] + \frac{N_c I_0}{4\pi^2} (\sigma_a^2 + \phi_a^2) \\ &- \frac{N_c I_1}{12\pi^2} \left\{ \left[2(M_u + M_d)^2 - M_u M_d - M_s^2 \right] (\sigma_1^2 + \sigma_2^2) \right. \\ &+ \left[2(M_u + M_s)^2 - M_u M_s - M_d^2 \right] (\sigma_4^2 + \sigma_5^2) \\ &+ \left[2(M_d + M_s)^2 - M_d M_s - M_u^2 \right] (\sigma_6^2 + \sigma_7^2) \\ &+ \frac{1}{2} [\sigma_u^2 (8M_u^2 - M_d^2 - M_s^2) + \sigma_d^2 (8M_d^2 - M_u^2 - M_s^2) \\ &+ \sigma_s^2 (8M_s^2 - M_u^2 - M_d^2)] \\ &+ \frac{1}{2} [\phi_u^2 (2M_u^2 - M_d^2 - M_s^2) + \phi_d^2 (2M_d^2 - M_u^2 - M_s^2) \\ &+ \phi_s^2 (2M_s^2 - M_u^2 - M_d^2)] \\ &+ \left. \left[2(M_u - M_d)^2 + M_u M_d - M_s^2 \right] (\phi_1^2 + \phi_2^2) \right\} \end{aligned}$$

$$\begin{aligned} &+ \left[2(M_u - M_s)^2 + M_u M_s - M_d^2 \right] (\phi_4^2 + \phi_5^2) \\ &+ \left[2(M_d - M_s)^2 + M_d M_s - M_u^2 \right] (\phi_6^2 + \phi_7^2) \\ &+ \frac{1}{2} h_{ab}^{(1)} \sigma_a \sigma_b + \frac{1}{2} h_{ab}^{(2)} \phi_a \phi_b. \end{aligned} \quad (24)$$

The kinetic term requires a redefinition of the meson fields,

$$\sigma_a = g\sigma_a^R, \quad \phi_a = g\phi_a^R, \quad g^2 = \frac{4\pi^2}{N_c I_1}, \quad (25)$$

to obtain the standard factor 1/4. The flavor and charged pseudoscalar fields are related through

$$\frac{\lambda_a}{\sqrt{2}} \phi_a = \begin{pmatrix} \frac{\phi_u}{\sqrt{2}} & \pi^+ & K^+ \\ \pi^- & \frac{\phi_d}{\sqrt{2}} & K^0 \\ K^- & \bar{K}^0 & \frac{\phi_s}{\sqrt{2}} \end{pmatrix} \quad (26)$$

and similarly for the scalar fields. In the following we concentrate on the diagonal components of (26), which according to eq. (7) induce mixing between the 0, 3, 8 field components of (24), in general. Indicating also the result of the transformations discussed below in (29), (30), we arrive at the following useful relations among fields

$$\begin{aligned} \phi_u &= \phi_3 + \frac{\sqrt{2}\phi_0 + \phi_8}{\sqrt{3}} = \phi_3 + \eta_{ns} \\ \phi_d &= -\phi_3 + \frac{\sqrt{2}\phi_0 + \phi_8}{\sqrt{3}} = -\phi_3 + \eta_{ns} \\ \phi_s &= \sqrt{\frac{2}{3}}\phi_0 - \frac{2\phi_8}{\sqrt{3}} = \sqrt{2}\eta_s. \end{aligned} \quad (27)$$

The neutral physical states π^0, η, η' are related to the 3×3 symmetric pseudoscalar meson mass matrix of elements B_{ij} emerging in the $i, j = \{0, 3, 8\}$ channels of L_{mass} by a sequence of two transformations $\mathcal{S} = \mathcal{U}\mathcal{V}$ that diagonalize it

$$(\phi_3, \phi_0, \phi_8) S^{-1} S \begin{pmatrix} B_{33} & B_{03} & B_{38} \\ B_{03} & B_{00} & B_{08} \\ B_{38} & B_{08} & B_{88} \end{pmatrix} S^{-1} S \begin{pmatrix} \phi_3 \\ \phi_0 \\ \phi_8 \end{pmatrix}, \quad (28)$$

first a rotation to the strange-nonstrange basis through the orthogonal involutory matrix \mathcal{V}

$$\begin{pmatrix} \phi_3 \\ \eta_{ns} \\ \eta_s \end{pmatrix} = \mathcal{V} \begin{pmatrix} \phi_3 \\ \phi_0 \\ \phi_8 \end{pmatrix} \quad (29)$$

with

$$\mathcal{V} = \frac{1}{\sqrt{3}} \begin{pmatrix} \sqrt{3} & 0 & 0 \\ 0 & \sqrt{2} & 1 \\ 0 & 1 & -\sqrt{2} \end{pmatrix}, \quad (30)$$

and then through the unitary transformation \mathcal{U} to the physical states [25]

$$\begin{pmatrix} \pi^0 \\ \eta \\ \eta' \end{pmatrix} = \mathcal{U}(\epsilon_1, \epsilon_2, \psi) \begin{pmatrix} \phi_3 \\ \eta_{ns} \\ \eta_s \end{pmatrix}, \quad (31)$$

where

$$\mathcal{U} = \begin{pmatrix} 1 & \epsilon_1 + \epsilon_2 \cos \psi & -\epsilon_2 \sin \psi \\ -\epsilon_2 - \epsilon_1 \cos \psi & \cos \psi & -\sin \psi \\ -\epsilon_1 \sin \psi & \sin \psi & \cos \psi \end{pmatrix} \quad (32)$$

The conventional definitions $\epsilon = \epsilon_2 + \epsilon_1 \cos \psi$, $\epsilon' = \epsilon_1 \sin \psi$ for the mixing angles are used in the tables. The unitary matrix \mathcal{U} has been linearized in the $\pi^0 - \eta$ and $\pi^0 - \eta'$ mixing angles $\epsilon_1, \epsilon_2 \sim \mathcal{O}(\delta)$, $\delta \ll 1$. This can be done because ϕ_3 couples weakly to the η_{ns} and η_s states, decoupling in the isospin limit, while the mixing for the $\eta - \eta'$ system is strong. Nevertheless we have tested numerically the linearization by obtaining also the exact Euler angles associated with the transformation (31), [60], the differences lying within the one to two percent level for the cases studied.

In the isospin limit \mathcal{U} in (32) leads to the 2×2 orthogonal transformation R_ψ

$$\begin{pmatrix} \eta \\ \eta' \end{pmatrix} = R_\psi \begin{pmatrix} \eta_{ns} \\ \eta_s \end{pmatrix}, \quad (33)$$

with

$$R_\psi = \begin{pmatrix} \cos \psi & -\sin \psi \\ \sin \psi & \cos \psi \end{pmatrix}, \quad (34)$$

We remind that the angle ψ is related to the mixing angle θ_p

$$\begin{pmatrix} \phi_R^0 \\ \phi_R^8 \end{pmatrix} = \begin{pmatrix} \cos \theta_p & -\sin \theta_p \\ \sin \theta_p & \cos \theta_p \end{pmatrix} \begin{pmatrix} \eta' \\ \eta \end{pmatrix}. \quad (35)$$

of the physical states η, η' in the singlet-octet renormalized basis states ϕ_R^0, ϕ_R^8 as $\psi = \theta_p + \arctan \sqrt{2}$, with the principal value of the angle θ_p comprised in the interval $-(\pi/4) \leq \theta_p \leq (\pi/4)$, for details please see Appendix B of [61] and [62].

We emphasize that one can freely choose among the different orthogonal bases to address the mixing of states. The reason it is convenient to adopt the strange-nonstrange basis is that it allows to infer whether the mixing-parameters are determined in a process independent way; in the context of ChPT it has been shown to be so if certain OZI violating processes are suppressed, [63],[25][54], and with the exception of those originating from topological effects due to the $U(1)_A$ anomaly. At this level of accuracy the decay constants follow the pattern of particle state mixing in this basis which is tantamount to

having a single mixing angle involved in the determination of the decay constants associated with the η and η' mesons. We show in the next subsection that our model fulfills this condition at the approximation considered.

At this point one should remind the reader how the model's $m_{\eta'}$ contains a term related with the topological vacuum susceptibility. The generalized NJL Lagrangian which combines the $U_A(1)$ breaking by the 't Hooft ($2N_f$) determinantal Lagrangian with the 4q and 8q interactions has been shown in [62] to be in correspondence with the Witten-Veneziano formula [64] which relates $m_{\eta'}$, in the large N_c limit of QCD with massive quarks, to the topological susceptibility χ_{YM} of pure Yang-Mills,

$$m_{\eta'}^2 + m_\eta^2 - 2m_K^2 = -\frac{6}{f_\pi^2} \chi_{YM}. \quad (36)$$

In our model the topological susceptibility is obtained in the large N_c limit as the following combination of model parameters

$$\chi_{YM} = \frac{\kappa}{4} \left(\frac{M}{2G} \right)^3. \quad (37)$$

The cutoff Λ , which is the approximate scale at which dynamical chiral symmetry breaking sets in, does not appear explicitly in the relation for χ_{YM} , only hidden in the constituent quark mass M . This expression shows a judicious interplay of the subleading in N_c counting $U_A(1)$ breaking parameter κ and the LO in N_c 4q coupling G , which combine in a relation that survives in the large N_c limit. This shows that the roles of chiral symmetry breaking and the breaking through the Adler Bell Jackiw anomaly are intertwined to equip η' with its large mass, which does not vanish in the chiral limit.

III b. Decay parameters

At the order of the heat kernel considered, we obtain the model's axial-vector current as [62] [88]

$$\begin{aligned} \mathcal{A}_\mu^a = & \\ & \frac{1}{4} \text{tr}[(\{\sigma^R + Mg^{-1}, \partial_\mu \phi^R\} - \{\partial_\mu \sigma^R, \phi^R\}) \lambda_a] + \mathcal{O}(b_3) \end{aligned} \quad (38)$$

in terms of the anti-commutators involving the bosonized and renormalized fields σ^R, ϕ^R (25) and the constituent quark mass matrix $M = M_a \lambda_a$. From here it is straightforward to calculate the matrix elements in the singlet-octet basis

$$\langle 0 | \mathcal{A}_\mu^a(0) | \phi_R^b \rangle = i f^{ab} p_\mu. \quad (39)$$

One has

$$\begin{aligned} f^{00} &= \frac{M_u + M_d + M_s}{3g}, & f^{11} = f^{22} = f^{33} &= \frac{M_u + M_d}{2g} \\ f^{88} &= \frac{M_u + M_d + 4M_s}{6g}, & f^{08} &= \frac{M_u + M_d - 2M_s}{3\sqrt{2}g} \end{aligned}$$

$$f^{03} = \sqrt{2}f^{38} = \frac{M_u - M_d}{\sqrt{6}g} \quad (40)$$

$$f^{44} = f^{55} = \frac{M_u + M_s}{2g}, \quad f^{66} = f^{77} = \frac{M_d + M_s}{2g}. \quad (41)$$

In particular one obtains $\langle 0 | \mathcal{A}_\mu^{1+i2}(0) | \pi(p) \rangle = i\sqrt{2}f_\pi p_\mu$ and $\langle 0 | \mathcal{A}_\mu^{4+i5}(0) | K(p) \rangle = i\sqrt{2}f_K p_\mu$ with $f_\pi = \frac{M_u + M_d}{2g}$ and $f_K = \frac{M_u + M_s}{2g}$, at the order of the heat kernel expansion considered.

The neutral axial vector currents can alternatively be taken in the strange non-strange basis (27)

$$\begin{aligned} \mathcal{A}_\mu^{ns} &= \sqrt{\frac{2}{3}}\mathcal{A}_\mu^0 + \sqrt{\frac{1}{3}}\mathcal{A}_\mu^8, \\ \mathcal{A}_\mu^s &= \sqrt{\frac{1}{3}}\mathcal{A}_\mu^0 - \sqrt{\frac{2}{3}}\mathcal{A}_\mu^8, \end{aligned} \quad (42)$$

for which one obtains the decay constants

$$\langle 0 | \mathcal{A}_\mu^\sigma(0) | \phi_R^\tau \rangle = i f^{\sigma\tau} p_\mu, \quad \{\sigma, \tau\} = \{3, ns, s\} \quad (43)$$

$$\begin{aligned} f^{ns} &= f^3 = \frac{M_u + M_d}{2g}, \quad f^s = \frac{M_s}{g}, \\ f^{3,ns} &= \frac{M_u - M_d}{2g}, \quad f^{3,s} = f^{ns,s} = 0, \end{aligned} \quad (44)$$

where f^3, f^{ns}, f^s are short-hand notations for $f^{3,3}, f^{ns,ns}, f^{s,s}$. The elements of (43) are collected in the following matrix

$$\mathcal{F} = \begin{pmatrix} f_\pi & zf_\pi & 0 \\ zf_\pi & f_\pi & 0 \\ 0 & 0 & f_s \end{pmatrix} \quad (45)$$

with $z = \frac{M_u - M_d}{M_u + M_d} = \frac{f^{3,ns}}{f_\pi}$ marking the departure from isospin symmetry. It is of the order of the ratio involving $\frac{f_u - f_d}{f_u + f_d} \sim \mathcal{O}(\delta)$, with $f_f = M_f/g$ the decay constants $\mathcal{F}_f = \text{diag}\{f_u, f_d, f_s\}$.

According to the idea behind the strange-nonstrange basis, the transformation to obtain the physical decay constants

$$\mathcal{F}_P = \mathcal{U}\mathcal{F}, \quad P = \{\pi^0, \eta, \eta'\}, \quad (46)$$

is the same that transforms the states, eq.(31). In the following we discuss how the observables obtained from our model Lagrangian fulfill this condition. In order to do so, it is convenient to express the meson mass Lagrangian \mathcal{L}_n of the neutral states in the flavor basis

$$\begin{aligned} \mathcal{L}_n = \sum_{i=u,d,s} & \left\{ \frac{1}{2} [(\partial_\mu \sigma_{iR})^2 + (\partial_\mu \phi_{iR})^2 + \mathcal{C}_i \sigma_{iR}^2 + \mathcal{B}_i \phi_{iR}^2] \right. \\ & \left. + \sum_{j=u,d,s} (\xi_{ij} \sigma_{iR} \sigma_{jR} + \zeta_{ij} \phi_{iR} \phi_{jR}) \right\} \end{aligned} \quad (47)$$

with

$$\begin{aligned} \mathcal{C}_i &= \frac{N_c I_0}{2\pi^2} g^2 - \frac{2}{3} \xi_i, \quad \mathcal{B}_i = \frac{N_c I_0}{2\pi^2} g^2 - \frac{2}{3} \zeta_i, \\ \xi_{ij} &= \frac{g^2}{2} h_{ab}^{(1)} e_{ai} e_{bj}, \quad \zeta_{ij} = \frac{g^2}{2} h_{ab}^{(2)} e_{ai} e_{bj}, \end{aligned} \quad (48)$$

where ξ_{ij}, ζ_{ij} are symmetric quantities. The quantities ζ_i are

$$\zeta_i = 2M_i^2 - M_j^2 - M_k^2, \quad i \neq j \neq k. \quad (49)$$

Inserting them in \mathcal{B}_i and using the gap equations (23), one obtains

$$\mathcal{B}_i = g^2 \frac{h_i}{M_i}. \quad (50)$$

Similar expressions can be obtained for the ξ_i, \mathcal{C}_i , but they are not needed in the following. The divergence of the axial current (38) reads in this basis

$$\partial_\mu \mathcal{A}_\mu^i = (\sigma_{iR} + \frac{M_i}{g}) \partial^2 \phi_{iR} - (\partial^2 \sigma_{iR}) \phi_{iR}. \quad (51)$$

Using now the equations of motion for the σ_{iR}, ϕ_{iR} fields

$$\begin{aligned} 0 &= \partial^2 \sigma_{iR} - \mathcal{C}_i \sigma_{iR} - (\xi_{ij} \sigma_{jR} + \xi_{ij} \sigma_{iR}) \\ 0 &= \partial^2 \phi_{iR} - \mathcal{B}_i \phi_{iR} - (\zeta_{ij} \phi_{jR} + \zeta_{ij} \phi_{iR}) \end{aligned} \quad (52)$$

one obtains for the matrix elements

$$\langle 0 | \partial_\mu \mathcal{A}_\mu^i | \phi_{jR} \rangle = \frac{M_i}{g} (\mathcal{B}_i \delta_{ij} + 2\zeta_{ij}), \quad (53)$$

which encode all the chiral and $U_A(1)$ symmetry breaking terms. The off-diagonal elements of the inverse matrix pertinent to ζ_{ij} are calculated to be

$$\zeta_{ij}^{-1} = \frac{1}{4} (h_k \kappa + 2m_k \kappa_2 + 2g_8 m_i m_j), \quad i \neq j \neq k. \quad (54)$$

These contributions violate the OZI rule, the ones proportional to κ, κ_2 have their origin in the $U_A(1)$ anomaly. The term $\sim g_8$ is a contribution of the order of the square of the current quark masses.

For comparison the transition elements of the divergence of the axial current in the strange non-strange basis are

$$Q_j^i = \langle 0 | \partial_\mu \mathcal{A}_\mu^i | \phi_{jR} \rangle, \quad i, j = \{3, ns, s\} \quad (55)$$

$$\begin{aligned} Q_3^3 &= \frac{f_\pi}{2} (b^+ + z(b^- - 2\zeta_{ud})) \\ Q_{ns}^3 &= \frac{f_\pi}{2} (b^- + z(b^+ + 2\zeta_{ud})) \\ Q_s^3 &= \frac{f_\pi}{\sqrt{2}} (\zeta_{us} - \zeta_{ds} + z(\zeta_{us} + \zeta_{ds})) \\ Q_3^{ns} &= \frac{f_\pi}{2} (b^- + z(b^+ - 2\zeta_{ud})) \end{aligned}$$

$$\begin{aligned}
Q_{ns}^{ns} &= \frac{f_\pi}{2}(b^+ + z(b^- + 2\zeta_{ud})) \\
Q_s^{ns} &= \frac{f_\pi}{\sqrt{2}}(\zeta_{us} + \zeta_{ds} + z(\zeta_{us} - \zeta_{ds})) \\
Q_3^s &= \frac{f_s}{\sqrt{2}}(\zeta_{us} - \zeta_{ds}), \quad Q_{ns}^s = \frac{f_s}{\sqrt{2}}(\zeta_{us} + \zeta_{ds}) \\
Q_s^s &= f_s\left(\frac{\mathcal{B}_s}{2} + \zeta_{ss}\right)
\end{aligned} \tag{56}$$

with

$$b^\pm = \left(\frac{\mathcal{B}_u}{2} + \zeta_{uu}\right) \pm \left(\frac{\mathcal{B}_d}{2} + \zeta_{dd}\right) \tag{57}$$

Note that the elements Q_j^i , $i, j = \{3, ns, s\}$ are not symmetric under exchange of $\{i, j\}$ differing by terms $\sim z$ and $\sim y = \frac{f_s}{f_\pi}$. Obviously in the isospin limit the elements $Q_3^3, Q_3^{ns}, Q_s^3, Q_s^s$ vanish. In this limit the $Q_{ns}^s = yQ_s^{ns}$, y being a measure for flavor breaking in the light vs. strange sector.

Finally using the relations (31),(32) and (56) we calculate the vacuum to physical particle transitions of the divergence of the axial current, $\langle 0 | \partial_\mu \mathcal{A}_\mu^b | P \rangle$, $b = \{3, ns, s\}$, $P = \{\pi^0, \eta, \eta'\}$, discarding terms $\sim \delta^2$, and are able to show that it fulfills the following relation [25]

$$\langle 0 | \partial_\mu \mathcal{A}_\mu^b | P_a \rangle = \mathcal{M}_{aa'}^2 \mathcal{U}_{a'b'} \mathcal{F}_{b'b}. \tag{58}$$

with \mathcal{F} given by (45) and $\mathcal{M}_{aa'}$ the physical meson mass matrix, which on the requirement of being diagonal determines the mixing angles $\psi, \epsilon, \epsilon'$. Thus the decay constants transform as the states (31) within our model calculations, at the order of the heat kernel considered. Higher order terms involve derivative interactions, which are likely to change this behavior.

We obtain the following relations at $\mathcal{O}(\delta)$

$$\begin{aligned}
\sum_{P=\pi^0, \eta, \eta'} f_P^3 f_P^3 &= f_\pi^2, \quad \sum_{P=\pi^0, \eta, \eta'} f_P^{ns} f_P^{ns} = f_\pi^2 \\
\sum_{P=\pi^0, \eta, \eta'} f_P^s f_P^s &= f_s^2,
\end{aligned} \tag{59}$$

for the diagonal elements, and

$$\begin{aligned}
\sum_{P=\pi^0, \eta, \eta'} f_P^{ns} f_P^s &= \sum_{P=\pi^0, \eta, \eta'} f_P^3 f_P^s = 0, \\
\sum_{P=\pi^0, \eta, \eta'} f_P^3 f_P^{ns} &= z f_\pi^2
\end{aligned} \tag{60}$$

for the crossed terms. The last relation is a consequence of (45). The vanishing of the other crossed terms indicates that just one mixing angle is present for the $\eta - \eta'$ mixing in the strange nonstrange basis at this order of approximation. This can be seen in a simple way in the isospin limit, and the argument is the same in the general

case. In the isospin limit the physical states $P = \eta, \eta'$ are now only mixtures of the nonstrange and strange components, as follows from (33). This case has been considered in [62] (where a detailed discussion of the mixing scheme in connection with the singlet octet basis in the isospin limit is also presented),

$$\langle 0 | \mathcal{A}_\mu^i(0) | P(p) \rangle = i f_P^i p_\mu, \quad (i = ns, s). \tag{61}$$

The couplings can be represented in a way which is similar to the one of Leutwyler – Kaiser [63],[54], who introduce two mixing angles $\vartheta_{ns}, \vartheta_s$

$$\{f_P^i\} = \begin{pmatrix} f_{ns}^{ns} & f_s^s \\ f_{\eta'}^{ns} & f_{\eta'}^s \end{pmatrix} = \begin{pmatrix} f_{ns} \cos \vartheta_{ns} & -f_s \sin \vartheta_s \\ f_{ns} \sin \vartheta_{ns} & f_s \cos \vartheta_s \end{pmatrix} \tag{62}$$

Our calculations show that within our model, with $M = M_u = M_d$,

$$\begin{aligned}
f_\eta^{ns} &= \frac{\bar{M}}{g} \cos \psi, & f_\eta^s &= -\frac{M_s}{g} \sin \psi, \\
f_{\eta'}^{ns} &= \frac{\bar{M}}{g} \sin \psi, & f_{\eta'}^s &= \frac{M_s}{g} \cos \psi.
\end{aligned} \tag{63}$$

One thus obtains the relation for the mixing angles

$$\sum_{P=\eta, \eta'} f_P^{ns} f_P^s = f^{ns} f^s \sin(\vartheta_{ns} - \vartheta_s) = 0. \tag{64}$$

This follows as the basic parameters $f_{ns}, f_s, \vartheta_{ns}, \vartheta_s$ of the matrix $\{f_P^i\}$, expressed in terms of model parameters (in the approximation considered)

$$f_{ns} = \frac{\bar{M}}{g} = f_\pi, \quad f_s = \frac{M_s}{g}, \quad \psi = \vartheta_{ns} = \vartheta_s. \tag{65}$$

There is a direct relation between the common mixing angle $\vartheta_{ns} = \vartheta_s$ and the OZI-rule which has been discussed in [63],[54]. The model predictions agree well with the general requirements of chiral symmetry following from chiral perturbation theory (ChPT), although the results differ already at lowest order. For instance, we have

$$f_s^2 = 2\bar{f}_K^2 - \bar{f}_\pi^2 + \frac{(M_s - \bar{M})^2}{2\bar{g}^2} \tag{66}$$

where barred quantities are a reminder that they are taken in the isospin limit. The first two terms of this formula are a well known low-energy relation which is valid in standard ChPT. In the η' -extended version of ChPT there is a OZI-rule violating term in the effective Lagrangian, which contributes as $\bar{f}_\pi^2 \Lambda_1$ to r.h.s. of (66). We have instead the term $(M_s - \bar{M})^2 / (2\bar{g}^2)$. Of course, in our case the origin of this contribution is related with the $SU(3)$ flavour symmetry breaking effect and does not have impact on the deviation from a single mixing angle in the strange-nonstrange basis reported as consequence of the OZI-rule violating parameter Λ_1 .

Away from the isospin limit one obtains

$$f_s^2 = 2f_K^2 - f_\pi^2(1 + 2z) + \frac{(M_s - M_u)^2}{2g^2}, \quad (67)$$

with a correction of order δ in the f_π^2 term, as compared to (66). The numerical values that we obtain are $z \sim 4 \times 10^{-3}$, which amounts to a small correction of $\sim 0.8\%$ in the f_π^2 term.

For completeness we indicate the decay constants and mixing angles in the singlet-octet basis in the isospin limit, used in Table (IV), for details see please [62],

$$\begin{aligned} \theta_0 &= \psi - \arctan(\sqrt{2} \frac{\bar{M}}{M_s}), \\ \theta_8 &= \psi - \arctan(\sqrt{2} \frac{M_s}{\bar{M}}) \\ \psi &= \theta_P + \arctan\sqrt{2} \end{aligned} \quad (68)$$

$$\begin{aligned} f_0^2 &= \frac{2\bar{f}_K^2 + \bar{f}_\pi^2}{3} + \frac{\bar{f}_\pi^2}{6} \left(\frac{M_s}{\bar{M}} - 1 \right)^2 \\ f_8^2 &= \frac{4\bar{f}_K^2 - \bar{f}_\pi^2}{3} + \frac{(M_s - \bar{M})^2}{3g^2} \end{aligned} \quad (69)$$

IV. Results and further discussion

The model has 15 parameters, 4 couplings G, κ, g_1, g_2 associated with L_{int} in (2), 7 non-vanishing couplings $\kappa_2, g_3, \dots, g_8$ in the ESB sector (4), the cutoff Λ , and the 3 current quark masses. Before running a fit it is convenient to understand to which parameters the difference of the light quark masses ($m_u - m_d$) is most sensitive. For that it is instructive to look at the matrix components (17) in the strange-nonstrange basis, which vanish in the isospin limit. As mentioned before these elements belong to the SPA contribution to the meson mass Lagrangian, see last line in (24), which is the part that carries the full information on the model couplings. Note that the heat kernel contribution to the meson masses, represented except for the kinetic terms in the remaining of expression (24), only depends on the cutoff Λ of the I_i quark integrals. The dependence on the model couplings of the heat kernel contribution only enters implicitly through the constituent quark masses, via the gap equations (23) which are solved selfconsistently with the lowest order SPA equations (16). Defining $m_\Delta = \frac{1}{2}(m_d - m_u)$, $m_\Sigma = \frac{1}{2}(m_d + m_u)$, $h_\Delta = \frac{1}{2}(h_d - h_u)$ and $h_\Sigma = \frac{1}{2}(h_d + h_u)$, one has for the inverse matrix elements of the ζ_{ij} matrix, $i, j = \{3, ns, s\}$

$$\begin{aligned} (\zeta_{3,ns})^{(-1)} &= \frac{1}{4} [h_\Delta(2g_2h_\Sigma + g_3m_\Sigma) \\ &+ m_\Delta(g_3h_\Sigma - 2(g_5 - g_6 + 2g_8)m_\Sigma)] \\ (\zeta_{3,s})^{(-1)} &= \frac{1}{2\sqrt{2}}(h_\Delta\kappa + 2m_\Delta(\kappa_2 - g_8m_s)) \end{aligned}$$

$$(\zeta_{ns,s})^{(-1)} = \frac{1}{2\sqrt{2}}(h_\Sigma\kappa + 2(\kappa_2 + g_8m_s)m_\Sigma). \quad (70)$$

The first two elements vanish in the isospin symmetric case. The third element relates to the mixing in $\eta - \eta'$ and is non-zero in this limit. In this basis one sees that the mixing in the $3, ns$ sector involves other couplings as in the strangeness related sectors, in contrast to the off-diagonal matrix elements in the u, d, s basis, (54). This sets new constraints on these couplings, as compared to the isospin symmetric case. It follows that the interplay of these parameters (which is conditioned by the fits), not the actual magnitude of each of the terms, is relevant to obtain the size of isospin corrections. We remark that in $(\zeta_{ns,s})^{(-1)}$ isospin breaking effects are absent, and that in the diagonal elements (not shown) they are overshadowed by the presence of $m_s, m_\Sigma, h_s, h_\Sigma$.

The current quark mass dependence in these expressions enters together with the ESB couplings. In their absence the effects of ESB come only through the difference in the light condensates h_Δ which do not vanish if the conventional QCD mass term has $m_u \neq m_d$ values, and if the couplings κ and g_2 are not zero (if they also vanish, only the heat kernel contribution to the meson mass matrix carries the effects of isospin breaking). The coupling κ is strongly correlated with the $\eta - \eta'$ mass splitting and it enters in the corresponding $(\zeta_{ns,s})^{(-1)}$ matrix element as factor of h_Σ which remains approximately constant. Thus this parameter is not expected to vary much in the fit of isospin breaking effects, which has been also verified numerically.

Before showing the results for isospin breaking, we display relevant model observables in the isospin limit, in comparison to other approaches. We consider the cases in which the ESB terms are present in the interaction Lagrangian, sets (a,b) in the Tables I-IV, and compare with the parameter set (c) in which explicit symmetry breaking occurs only through the LO current quark mass term. Table I indicates the mass spectra of the low lying pseudoscalar (and scalar meson nonets, see caption, for sets (a,b)) used in the fit of parameters. Sets (a,b) have different mixing angles for the pseudoscalars as well as for the scalars, leaving however the mass spectra and weak decay constants f_π, f_K unchanged. This is possible because the fit is done simultaneously in both sectors, leading to a readjustment of parameters. A comment on the scalar mass spectrum: we were able to obtain a reasonable simultaneous fit for the σ mass and its large decay width, at tree level of the mesonic Lagrangian. It is our understanding that this results partly from the fact that already at mesonic tree level there are signatures of quark-antiquark as well as of admixtures of 2 quark-2 antiquark states present, from the underlying multi-quark Lagrangian, which contribute in the long distance asymptotics to the internal structure of the mesons as well as to the mesonic interaction terms. In many other

approaches the more complex quark structures enter only through the explicit inclusion of meson loops, tetraquark configurations, and so on [65–77].

Table II shows the current and constituent quark masses in the isospin limit and the model parameters which do not break explicitly the chiral symmetry, the 4-quark coupling G , the 6-quark t Hooft determinant coupling κ , and two 8-quark couplings g_1, g_2 , of which g_1 is OZI-violating. In set (c) we put $g_1 = 2500$ without loss of generality, since a change in g_1 can be counterbalanced by a change in G leaving all other parameters and observables unchanged, except for the low lying σ -meson mass, see e.g. [62], [78], which does not affect the pseudoscalar characteristics considered here. Table III displays the couplings related with the ESB interactions.

In Table IV further properties of the $\eta - \eta'$ system are presented, the angle θ_P in the singlet-octet basis and the related angles θ_0, θ_8 , as well as the weak decays f_0, f_8 , see eqs. (68),(69) obtained following the methods in sections 3.2 and 3.3 of [62], and compared with the results of other approaches [22] and references therein, [79], [54],[80], and of Padé approximant method to pseudoscalar transition form factors [82], [81], where in the Table IV, (η) and (η') refer to the asymptotes taken for the fits, and the results obtained from BABAR data [83] by the same authors (see discussion in [81] concerning the BABAR "puzzle").

This comparison shows that set (a) yields results quite close to the chiral perturbation analysis of [79] and follows the general trend of the other references in the table, with exception of the sum rules approach of [80], and the fits from [83]. Our values for θ_0, θ_8 are smaller, respectively larger than the ones presented in [22], which is probably due to the different way in which the $U(1)_A$ anomaly is treated. One further notices that an increase in θ_P leads mainly to an increase in the θ_0 angle, comparing sets (a) and (b), which have similar theoretical input.

Turning now to isospin breaking, in the numerical fit we keep the cutoff Λ , which sets approximately the scale of chiral symmetry breaking, close to the isospin limit value, and take for the strange current quark mass the value $m_s = 95$ MeV. We do not consider the scalar spectrum in this case, the related isospin breaking effects will be addressed in a future work. Then the general case, with the ESB terms, involves solving self-consistently a system of 13 equations, the three gap equations (23) subject to the three SPA conditions (16), 6 equations for the meson mass matrix elements, that is 3 for $m_{\pi^0}, m_\eta, m_{\eta'}$ and the remaining 3 for diagonalization, one equation for the kaon mass, 2 equations for the weak decay constants f_π, f_K , one equation which fixes the ratio $r = \frac{m_d - m_u}{m_u + m_d}$ of current quark masses. We vary externally the values of the mixing angles $\epsilon, \epsilon', \psi$ and search for the parameters

that lead to the best fit of the m_u, m_d current masses. The result is indicated in Table VII, using empirical input and couplings shown in Tables V and VI (the empirical splitting of the charged multiplets cannot be reproduced, since electromagnetic effects are not taken into account). In presence of ESB (sets A and B) with the ratio r kept equal and close to its empirical value, the ratio $\frac{\epsilon}{\epsilon'}$ is well reproduced in comparison with the literature shown in Table VIII. The main observation is that this ratio is reduced by $\sim 40\%$ compared to the model variant without ESB interactions, set C. In the latter case one does not obtain $\frac{\epsilon}{\epsilon'}$ nor m_u, m_d close to the empirical values. Neither this ratio nor the light current quark masses get improved in set C by reducing r down to 0.2, the main consequence being a drastic change in the values for the mixing angles, which get reduced to $\epsilon = 0.0119, \epsilon' = 0.00135$. We note that it is not possible to get a better fit for m_η, m_K and f_K in absence of ESB interactions as the one shown in set C in Table V. Contrary to this, the individual values for ϵ and ϵ' for sets A,B are in good agreement with the ones indicated in [63], [25] and the corresponding current quark masses are very close to the quoted values $m_u = 2.15(15)$ MeV, $m_d = 4.70(20)$ MeV, [87].

Regarding table VIII that collects values obtained in the literature, within different phenomenological approaches, as well as in experiments, a comparison of the different values has to be done with care, for a careful and detailed discussion see [25]. We note in particular that in the experimental value [86] the mixing $\pi^0 - \eta'$ has not been taken into account and that in the ChPT result [79] the η' is considered as a background field.

V. Concluding remarks

We conclude that the explicit symmetry breaking interactions of the generalized NJL Lagrangian considered are crucial to obtain the phenomenological quoted value for the ratio $\frac{\epsilon}{\epsilon'}$. We obtain values for the ϵ mixing angle which lie within the results discussed in the literature. Unfortunately the value for ϵ' is much less discussed. We obtain ϵ and ϵ' reasonably close to the ones indicated in [63], [25] for current quark mass values in excellent agreement with the presently quoted average values. The corresponding sets (A,B) are the ones which also yield the best fits to other empirical data within the model variants.

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